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Vibrational Energy Transfer

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FINAL REPORT

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PERIOD COVERED BY REPORT: August 15, 1977 - March 31, 1981

TITLE OF PROPOSAL: Laser Studies of Molecular Collision Processes

CONTRACT OR GRANT NUMBER: DAAG26-77-G-0200

NAME OF INSTITUTION: Department of Chemistry
University of California
Berkeley, CA 94720

PRINCIPAL INVESTIGATOR: Professor C. Bradley Moore

I. Statement of Problem:

The purpose of this research has been to determine the effect of selective electronic and vibrational excitation on energy transfer and reaction rates in simple molecular systems.

II. Principal Results:

A wide variety of behavior is exhibited in the competition between reaction and energy transfer for simple molecular systems. The principal results can be grouped into 3 categories.

(1) Relaxation of highly vibrationally excited species

The competition between relaxation and reaction in collisions of a highly vibrationally excited diatomic with thermal molecules has been studied. The observation of multiquantum energy transfer upon collision infers the occurrence of a reaction. In studies of HF(v = 4) with a variety of collision partners, removal of the initially excited species is seen to occur via single quantum energy transfer implying that the relaxation channel dominates.

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cont (2) Vibrational Relaxation in Polyatomic Systems

Studies of vibrational relaxation pathways have been extended to the CH_4, NH_3, H_2O, D_2O, H_2Se, D_2S systems. It is shown that systems which interact via hydrogen bonding show increased $V \rightarrow T, R$ rates with negative temperature dependence near room temperature. The enhanced $V \rightarrow T, R$ rates and negative temperature dependence can be explained with a model in which orbiting collisions are most effective in causing relaxation.

3) Vibrational Relaxation in Condensed Media

The vibrational spectroscopy and dynamics of matrix isolated HCl and CH_3F have been studied. At the cryogenic temperatures of these experiments, the attractive part of the intermolecular guest-host potential is seen to play an increasingly important role in causing vibrational relaxation. For those systems in which the attractive forces are known to be strong, as evidenced by the existence of van-der-Waals molecules in the gas phase, i.e. HCl-rare gas, relaxation rates correlate well with increasing intermolecular well depth. In all systems studied, there is a marked dependence of relaxation rates on host, spanning two orders of magnitude between Ar and Xe.

III. Publications:

C.C. Mei and C.B. Moore, Temperature Dependence of the Total Reaction Rates for Cl + HI and Cl + HBr, J. Chem. Phys. 67, 3936 (1977).

J. Finzi, F.E. Hovis, V.N. Panfilov, P. Hess, and C.B. Moore, Vibrational Relaxation of Water Vapor, J. Chem. Phys. 67, 4053 (1977).

R.G. Macdonald and C.B. Moore, Reaction and Deactivation of HCl(v = 1,2) by O atoms, J. Chem. Phys. 68, 513 (1978).

D.J. Douglas and C.B. Moore, Vibrational Relaxation of HF(v = 3,4), Chem. Phys. Lett. 57, 485 (1978).

F.E. Hovis and C.B. Moore, Vibrational Relaxation of $NH_3(\nu_2)$, J. Chem. Phys. 69, 4947 (1978).

J.M. Wiesenfeld and C.B. Moore, Vibrational Relaxation of Matrix Isolated HCl and DCl, J. Chem. Phys. 70, 930 (1979).

D.J. Douglas and C.B. Moore, Vibrational Relaxation of HF(v = 3,4) by H_2, D_2, and CO_2, J. Chem. Phys. 70, 1769 (1979).

C.C. Mei and C.B. Moore, Thermal Rate Constants, Energy Dependence, and Isotope Effect for Halogen-Hydrogen Halide Reactions, J. Chem. Phys. 70, 1759 (1979).

P. Hess and C.B. Moore, Study of Energy Transfer in Methane by Excitation of Fundamental, Overtone, and Combination Bands, Laser-Induced Processes in Molecules, eds. K.L. Kompa and S.D. Smith. Proceedings of the European Physical Society Divisional Conference, Edinburgh, Scotland, 1978, p. 339.

D.J. Douglas and C.B. Moore, Vibrational Relaxation of HF(v = 3,4) by HF, H_2, D_2, CO_2, and Isobutene, Laser-Induced Processes in Molecules, eds. K.L. Kompa and S.D. Smith. Proceedings of the European Physical Society Divisional Conference, Edinburgh, Scotland, 1978, p. 336.

P. Ho and C.B. Moore, Laser Separation of Isotopes by Photopredissociation, Proceedings of the First National School "Laser Application in Atomic, Molecular and Nuclear Physics", Vilnius, U.S.S.R., August 1978.

F.E. Hovis and C.B. Moore, Energy Transfer and Laser Photochemistry, Proceedings of the First National School "Laser Application in Atomic, Molecular and Nuclear Physics", Vilnius, U.S.S.R., August 1978.

III. Publications: (continued)

S.J. Harris, W.C. Natzle, and C.B. Moore, Zero Pressure Lifetimes and Fluorescence Quenching of $ICl(A^3\Pi_1)$, J. Chem. Phys. 70, 4215 (1979).

H.-L. Dai, A.H. Kung, and C.B. Moore, Resonant Multiphoton Dissociation and Mechanism of Excitation for Ethyl Chloride, Phys. Rev. Lett. 43, 761 (1979).

C.B. Moore and I.W.M. Smith, Vibrational-Rotational Excitation - Chemical Reactions of Vibrationally Excited Molecules, Faraday Disc. Chem. Soc. 67, 146 (1979).

A.H. Kung, H.-L. Dai, M.R. Berman, and C.B. Moore, Resonant Multiphoton Dissociation of Small Molecules in Laser Spectroscopy IV, eds. H. Walther et al., Proceedings of the Fourth International Conference on Laser Spectroscopy, Rottach-Egern, West Germany, Springer-Verlag 1979, p. 309.

C.J. Dasch and C.B. Moore, Single Quantum Vibrational Energy Transfer from HCl ($v = 2$) and HBr ($v = 2$), J. Chem. Phys. 72, 4117 (1980).

C.J. Dasch and C.B. Moore, Experimental V $\rightarrow$ V Energy Transfer from Directly Excited CO($v = 2$) and DCl($v = 2$), J. Chem. Phys. 72, 5219 (1980).

P. Hess, A.H. Kung, and C.B. Moore, Vibration $\rightarrow$ Vibration Energy Transfer in Methane, J. Chem. Phys. 72, 5525 (1980).

S.S. Miljanic and C.B. Moore, Vibrational Relaxation of $D_2O(\nu_2)$, J. Chem. Phys. 73, 226 (1980).

R.G. Macdonald and C.B. Moore, Reaction and Deactivation of HCl($v = 1,2$) by Cl, Br, and H atoms, J. Chem. Phys. 73, 1681 (1980).

J.S. Wong and C.B. Moore, Bond Selective Excitation of Molecules, Lasers and Applications, eds. W.O.N. Guimaraes, C.-T. Lin, and A. Mooradian. Proceedings of the Sergio Porto Memorial Symposium, Rio de Janeiro, Brazil, 1980, Springer Verlag 1981, p. 157.

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